

1-Phenylurea
64-10-8 | DTXSID8042507

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 4.53 days

Global applicability domain: Outside

Local applicability domain index: 3.40e-01

Confidence level: 8.75e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Propylbenzene</div> <div>Measured: 24.3</div> <div>Predicted: 4.02</div>	<div>Image not found</div> <div>4-Ethyltoluene</div> <div>Measured: 24.3</div> <div>Predicted: 3.95</div>	<div>Image not found</div> <div>Ethylbenzene</div> <div>Measured: 120</div> <div>Predicted: 6.21</div>
<div>Image not found</div> <div>1-Methyl-2-propylbenzene</div> <div>Measured: 12.5</div> <div>Predicted: 3.17</div>	<div>Image not found</div> <div>1,2-Dimethyl-4-ethylbenzene</div> <div>Measured: 40.7</div> <div>Predicted: 4.08</div>	